Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:ssptaeal1624

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS 1		Web Page for STN Seminar Schedule - N. America
NEWS 2	NOV 21	CAS patent coverage to include exemplified prophetic substances identified in English-, French-, German-, and Japanese-language basic patents from 2004-present
NEWS 3	NOV 26	MARPAT enhanced with FSORT command
NEWS 4	NOV 26	CHEMSAFE now available on STN Easy
NEWS 5	NOV 26	Two new SET commands increase convenience of STN searching
NEWS 6	DEC 01	ChemPort single article sales feature unavailable
NEWS 7	DEC 12	GBFULL now offers single source for full-text coverage of complete UK patent families
NEWS 8	DEC 17	Fifty-one pharmaceutical ingredients added to PS
NEWS 9	JAN 06	The retention policy for unread STNmail messages will change in 2009 for STN-Columbus and STN-Tokyo
NEWS 10	JAN 07	WPIDS, WPINDEX, and WPIX enhanced Japanese Patent Classification Data
NEWS 11	FEB 02	Simultaneous left and right truncation (SLART) added for CERAB, COMPUAB, ELCOM, and SOLIDSTATE
NEWS 12	FEB 02	GENBANK enhanced with SET PLURALS and SET SPELLING
NEWS 13	FEB 06	Patent sequence location (PSL) data added to USGENE
NEWS 14	FEB 10	COMPENDEX reloaded and enhanced
NEWS 15	FEB 11	WTEXTILES reloaded and enhanced
NEWS 16	FEB 19	New patent-examiner citations in 300,000 CA/CAplus patent records provide insights into related prior art
NEWS 17	FEB 19	Increase the precision of your patent queries -- use terms from the IPC Thesaurus, Version 2009.01
NEWS 18	FEB 23	Several formats for image display and print options discontinued in USPATFULL and USPAT2
NEWS 19	FEB 23	MEDLINE now offers more precise author group fields and 2009 MeSH terms
NEWS 20	FEB 23	TOXCENTER updates mirror those of MEDLINE - more precise author group fields and 2009 MeSH terms
NEWS 21	FEB 23	Three million new patent records blast AEROSPACE into STN patent clusters
NEWS 22	FEB 25	USGENE enhanced with patent family and legal status display data from INPADOCDB
NEWS 23	MAR 06	INPADOCDB and INPAFAMDB enhanced with new display formats

NEWS EXPRESS JUNE 27 08 CURRENT WINDOWS VERSION IS V8.3,

AND CURRENT DISCOVER FILE IS DATED 23 JUNE 2008.

NEWS HOURS STN Operating Hours Plus Help Desk Availability
NEWS LOGIN Welcome Banner and News Items
NEWS IPC8 For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that specific topic.

All use of STN is subject to the provisions of the STN Customer agreement. Please note that this agreement limits use to scientific research. Use for software development or design or implementation of commercial gateways or other similar uses is prohibited and may result in loss of user privileges and other penalties.

* * * * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 16:23:34 ON 10 MAR 2009

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.44	0.44

FILE 'REGISTRY' ENTERED AT 16:24:30 ON 10 MAR 2009
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 9 MAR 2009 HIGHEST RN 1118246-54-0
DICTIONARY FILE UPDATES: 9 MAR 2009 HIGHEST RN 1118246-54-0

New CAS Information Use Policies, enter HELP USAGETERMS for details.

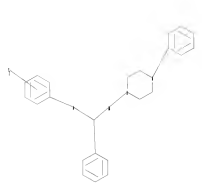
TSCA INFORMATION NOW CURRENT THROUGH January 9, 2009.

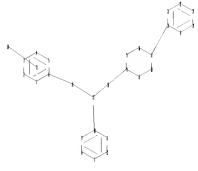
Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Program Files\Stnexp\Queries\10594105restriction.str





chain nodes :
25 26 27 30
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23
24
chain bonds :
6-25 10-27 14-26 17-20 25-27 26-27
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 13-14 13-18
14-15 15-16 16-17 17-18 19-20 19-24 20-21 21-22 22-23 23-24
exact/norm bonds :
6-25 13-14 13-18 14-15 14-26 15-16 16-17 17-18 17-20 25-27 26-27
exact bonds :
10-27
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 19-20 19-24
20-21 21-22 22-23 23-24
isolated ring systems :
containing 1 : 7 : 13 : 19 :

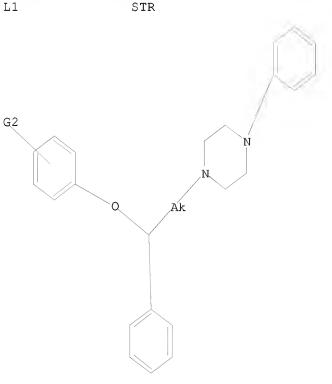
G1:C,N

G2:CF2,CF3,CCl2,CCl3,CBr2,CBr3,X

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
20:Atom 21:Atom 22:Atom 23:Atom 24:Atom 25:CLASS 26:CLASS 27:CLASS 30:CLASS
31:Atom

L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR



G1 C,N
G2 CF2,CF3,CCl2,CCl3,CBr2,CBr3,X

Structure attributes must be viewed using STN Express query preparation.

=> s l1 full
FULL SEARCH INITIATED 16:25:28 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 10796 TO ITERATE

100.0% PROCESSED 10796 ITERATIONS 116 ANSWERS
SEARCH TIME: 00.00.02

L2 116 SEA SSS FUL L1

=> file caplus
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 186.36 186.80

FILE 'CAPLUS' ENTERED AT 16:25:35 ON 10 MAR 2009

FILE COVERS 1907 - 10 Mar 2009 VOL 150 ISS 11
FILE LAST UPDATED: 9 Mar 2009 (20090309/ED)

Caplus now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2008.

CAS Information Use Policies apply and are available at:

http://www.cas.org/legal/infopolicy.html

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l2 full
L3 10 L2

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	1.50	188.30

FILE 'REGISTRY' ENTERED AT 16:27:34 ON 10 MAR 2009

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 9 MAR 2009 HIGHEST RN 1118246-54-0
DICTIONARY FILE UPDATES: 9 MAR 2009 HIGHEST RN 1118246-54-0

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 9, 2009.

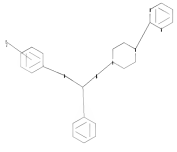
Please note that search-term pricing does apply when conducting SmartSELECT searches.

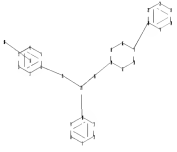
REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information

on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Program Files\Stnexp\Queries\10594105pyrimidine.str





chain nodes :
25 26 27 30
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23
24
chain bonds :
6-25 10-27 14-26 17-20 25-27 26-27
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 13-14 13-18
14-15 15-16 16-17 17-18 19-20 19-24 20-21 21-22 22-23 23-24
exact/norm bonds :
6-25 13-14 13-18 14-15 14-26 15-16 16-17 17-18 17-20 25-27 26-27
exact bonds :
10-27
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 19-20 19-24
20-21 21-22 22-23 23-24
isolated ring systems :
containing 1 : 7 : 13 : 19 :

G1:C,N

G2:CF2,CF3,CCl2,CCl3,CBr2,CBr3,X

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
20:Atom 21:Atom 22:Atom 23:Atom 24:Atom 25:CLASS 26:CLASS 27:CLASS 30:CLASS
31:Atom

L4 STRUCTURE UPLOADED

=> d l4
L4 HAS NO ANSWERS
L4 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

=> d l4
L4 HAS NO ANSWERS
L4 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

=> s l4 full
FULL SEARCH INITIATED 16:28:23 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 267 TO ITERATE

100.0% PROCESSED 267 ITERATIONS 6 ANSWERS
SEARCH TIME: 00.00.01

L5 6 SEA SSS FUL L4

=> file caplus
COST IN U.S. DOLLARS

	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	185.88	374.18

FILE 'CAPLUS' ENTERED AT 16:28:26 ON 10 MAR 2009
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 10 Mar 2009 VOL 150 ISS 11
FILE LAST UPDATED: 9 Mar 2009 (20090309/ED)

Caplus now includes complete International Patent Classification (IPC)
reclassification data for the third quarter of 2008.

CAS Information Use Policies apply and are available at:

http://www.cas.org/legal/infopolicy.html

This file contains CAS Registry Numbers for easy and accurate
substance identification.

=> s l5 full
L6   6 L5

=> file reg
COST IN U.S. DOLLARS   SINCE FILE   TOTAL
                                                         ENTRY   SESSION
FULL ESTIMATED COST   2.00   376.18

FILE 'REGISTRY' ENTERED AT 16:30:33 ON 10 MAR 2009
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES: 9 MAR 2009 HIGHEST RN 1118246-54-0
DICTIONARY FILE UPDATES: 9 MAR 2009 HIGHEST RN 1118246-54-0

New CAS Information Use Policies, enter HELP USAGETERMS for details.

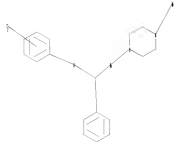
TSCA INFORMATION NOW CURRENT THROUGH January 9, 2009.

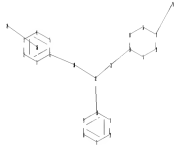
  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Program Files\Stnexp\Queries\10594105methyl.str





chain nodes :
19 20 21 22 25
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18
chain bonds :
6-20 10-22 14-21 17-19 20-22 21-22
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 13-14 13-18
14-15 15-16 16-17 17-18
exact/norm bonds :
6-20 13-14 13-18 14-15 14-21 15-16 16-17 17-18 17-19 20-22 21-22
exact bonds :
10-22
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12

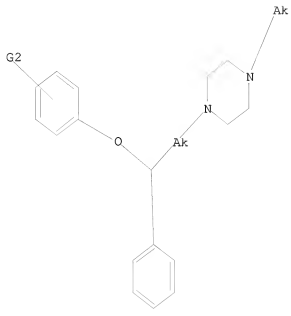
G1:C,N

G2:CF2,CF3,CCl2,CCl3,CBr2,CBr3,X

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
20:CLASS 21:CLASS 22:CLASS 25:CLASS 26:Atom

L7 STRUCTURE UPLOADED

```
=> d l7
L7 HAS NO ANSWERS
L7              STR
```




```
G1 C,N
G2 CF2,CF3,CCl2,CCl3,CBr2,CBr3,X


Structure attributes must be viewed using STN Express query preparation.


=> s l7 full
FULL SEARCH INITIATED 16:31:06 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -    69180 TO ITERATE

100.0% PROCESSED    69180 ITERATIONS                                74 ANSWERS
SEARCH TIME: 00.00.02

L8           74 SEA SSS FUL L7

=> file caplus
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                      ENTRY    SESSION
FULL ESTIMATED COST                                  185.88     562.06

FILE 'CAPLUS' ENTERED AT 16:31:15 ON 10 MAR 2009
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2009 AMERICAN CHEMICAL SOCIETY (ACS)


Copyright of the articles to which records in this database refer is
held by the publishers listed in the PUBLISHER (PB) field (available
```

for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 10 Mar 2009 VOL 150 ISS 11
FILE LAST UPDATED: 9 Mar 2009 (20090309/ED)

Caplus now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2008.

CAS Information Use Policies apply and are available at:

http://www.cas.org/legal/infopolicy.html

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l8 full
L9 8 L8

=> file reg
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 2.50 564.56

FILE 'REGISTRY' ENTERED AT 16:34:04 ON 10 MAR 2009
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2009 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 9 MAR 2009 HIGHEST RN 1118246-54-0
DICTIONARY FILE UPDATES: 9 MAR 2009 HIGHEST RN 1118246-54-0

New CAS Information Use Policies, enter HELP USAGETERMS for details.

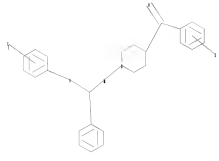
TSCA INFORMATION NOW CURRENT THROUGH January 9, 2009.

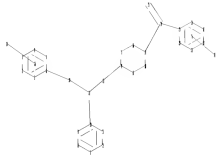
Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Program Files\Stnexp\Queries\10594105piperidine.str





chain nodes :
19 20 21 22 25 33 34
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 27 28 29 30 31
32
chain bonds :
6-20 10-22 14-21 17-19 19-29 19-33 20-22 21-22
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 13-14 13-18
14-15 15-16 16-17 17-18 27-28 27-32 28-29 29-30 30-31 31-32
exact/norm bonds :
6-20 13-14 13-18 14-15 14-21 15-16 16-17 17-18 19-33 20-22 21-22
exact bonds :
10-22 17-19 19-29
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 27-28 27-32
28-29 29-30 30-31 31-32
isolated ring systems :
containing 27 :

G1:C,N

G2:CF2,CF3,CCl2,CCl3,CBr2,CBr3,X

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
20:CLASS 21:CLASS 22:CLASS 25:CLASS 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom
31:Atom 32:CLASS 33:CLASS 34:CLASS 35:Atom

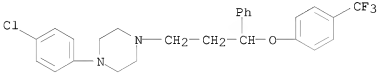
```
L10     STRUCTURE UPLOADED

=> s l10 full
FULL SEARCH INITIATED 16:34:52 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -      847 TO ITERATE

100.0% PROCESSED      847 ITERATIONS                                 6 ANSWERS
SEARCH TIME: 00.00.01

L11           6 SEA SSS FUL L10

=> file caplus
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                   186.36     750.92

FILE 'CAPLUS' ENTERED AT 16:35:00 ON 10 MAR 2009
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2009 AMERICAN CHEMICAL SOCIETY (ACS)


Copyright of the articles to which records in this database refer is
held by the publishers listed in the PUBLISHER (PB) field (available
for records published or updated in Chemical Abstracts after December
26, 1996), unless otherwise indicated in the original publications.
The CA Lexicon is the copyrighted intellectual property of the
American Chemical Society and is provided to assist you in searching
databases on STN.  Any dissemination, distribution, copying, or storing
of this information, without the prior written consent of CAS, is
strictly prohibited.

FILE COVERS 1907 - 10 Mar 2009  VOL 150 ISS 11
FILE LAST UPDATED: 9 Mar 2009  (20090309/ED)

Caplus now includes complete International Patent Classification (IPC)
reclassification data for the third quarter of 2008.

CAS Information Use Policies apply and are available at:

http://www.cas.org/legal/infopolicy.html

This file contains CAS Registry Numbers for easy and accurate
substance identification.

=> s l11 full
L12           2 L11

=> s l12 or l9 or l6 or l3
L13          16 L12 OR L9 OR L6 OR L3

=> d ibib abs hitstr tot
```

L13 ANSWER 1 OF 16 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2008:803320 CAPLUS
DOCUMENT NUMBER: 149:215113
TITLE: Two-dimensional QSAR studies on arylpiperazines as high-affinity 5-HT1A receptor ligands
AUTHOR(S): Weber, Karen C.; Honorio, Kathia M.; Andricopulo, Adriano D.; Da Silva, Alberico B. F.
CORPORATE SOURCE: Instituto de Quimica de Sao Carlos, Universidade de Sao Paulo, Sao Carlos, 13560-970, Brazil
SOURCE: Medicinal Chemistry (2008), 4(4), 328-335
CODEN: MCEHAJ; ISSN: 1573-4064
PUBLISHER: Bentham Science Publishers Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

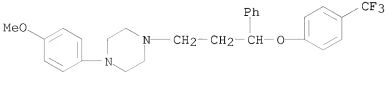
AB 5-HT1A receptor plays an important role in the delayed onset of antidepressant action of a class of selective serotonin reuptake inhibitors. Moreover, 5-HT1A receptor levels have been shown to be altered in patients suffering from major depression. In this work, hologram quant. structure-activity relationship (HQSAR) studies were performed on a series of arylpiperazine compds. presenting affinity to the 5-HT1A receptor. The models were constructed with a training set of 70 compds. The most significant HQSAR model (q2 = 0.81, r2 = 0.96) was generated using atoms, bonds, connections, chirality, and donor and acceptor as fragment distinction, with fragment size of 6-9. Predictions for an external test set containing 20 compds. are in good agreement with exptl. results showing the robustness of the model. Addnl., useful information can be obtained from the 2D contribution maps.

IT 328248-15-3 328248-21-1 328248-23-3
328248-24-4 328248-30-2 328248-36-8
753439-74-6 767277-20-3 777843-82-0
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(two-dimensional QSAR studies on arylpiperazines as high-affinity 5-HT1A receptor ligands)

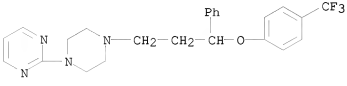
RN 328248-15-3 CAPLUS
CN Piperazine, 1-(4-chlorophenyl)-4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]- (CA INDEX NAME)



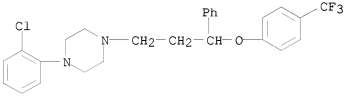
RN 328248-21-1 CAPLUS
CN Piperazine, 1-(4-methoxyphenyl)-4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]- (CA INDEX NAME)



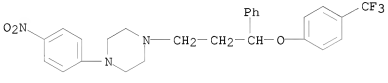
RN 328248-23-3 CAPLUS
CN Pyrimidine, 2-[4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]-1-piperazinyl]- (CA INDEX NAME)



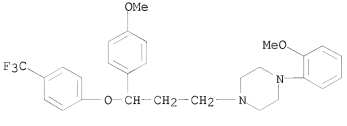
RN 328248-24-4 CAPLUS
CN Piperazine, 1-(2-chlorophenyl)-4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]- (CA INDEX NAME)



RN 328248-30-2 CAPLUS
CN Piperazine, 1-(4-nitrophenyl)-4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]- (CA INDEX NAME)

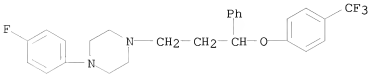


RN 328248-36-8 CAPLUS
CN Piperazine, 1-(2-methoxyphenyl)-4-[3-(4-methoxyphenyl)-3-[4-(trifluoromethyl)phenoxy]propyl]- (CA INDEX NAME)

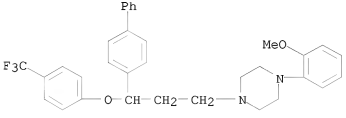


RN 753439-74-6 CAPLUS
CN Piperazine, 1-(4-fluorophenyl)-4-[3-phenyl-3-[4-

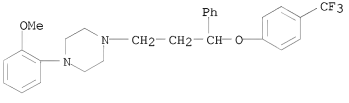
(trifluoromethyl)phenoxy]propyl]- (CA INDEX NAME)



RN 767277-20-3 CAPLUS
CN Piperazine, 1-[3-[1,1'-biphenyl]-4-yl-3-[4-(trifluoromethyl)phenoxy]propyl]-4-(2-methoxyphenyl)- (CA INDEX NAME)



RN 777843-82-0 CAPLUS
CN Piperazine, 1-(2-methoxyphenyl)-4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]- (CA INDEX NAME)



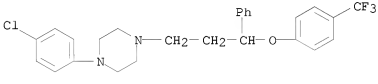
REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 2 OF 16 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2008:767635 CAPLUS
DOCUMENT NUMBER: 149:324283
TITLE: Quantitative structure-affinity relationship of 5-HT1A receptor ligands by the classification tree method
AUTHOR(S): Kuz'min, V. E.; Polischuk, P. G.; Artemenko, A. G.; Makan, S. Yu.; Andronati, S. A.
CORPORATE SOURCE: A.V. Bogatsky Physical-Chemical Institute, National Academy of Sciences of Ukraine, Odessa, Ukraine
SOURCE: SAR and QSAR in Environmental Research (2008), 19(3-4), 213-244
CODEN: SQERED; ISSN: 1062-936X
PUBLISHER: Taylor & Francis Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

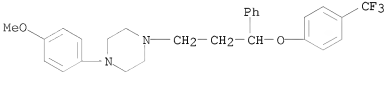
AB The influence of mol. structure of 346 ligands on their affinity for 5-HT1A receptors was investigated. It was shown that the effectiveness of the proposed novel approach for interpretation of decision tree models compared favorably with the PLS method. In the context of the proposed approach, mol. fragments and their values of the relative influence on the affinity for 5-HT1A receptors were defined.

IT 328248-15-3 328248-21-1 328248-23-3
328248-24-4 328248-30-2 328248-36-8
753439-74-6 767277-20-3 777843-82-0
RL: ANT (Analyte); BSU (Biological study, unclassified); PRP (Properties); ANST (Analytical study); BIOL (Biological study)
(quant. structure-affinity relationship of 5-HT1A receptor ligands by the classification tree method)

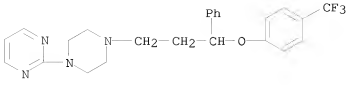
RN 328248-15-3 CAPLUS
CN Piperazine, 1-(4-chlorophenyl)-4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]- (CA INDEX NAME)



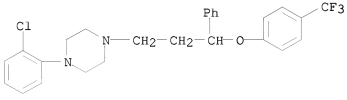
RN 328248-21-1 CAPLUS
CN Piperazine, 1-(4-methoxyphenyl)-4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]- (CA INDEX NAME)



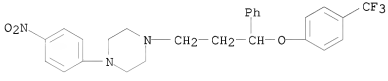
RN 328248-23-3 CAPLUS
CN Pyrimidine, 2-[4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]-1-piperazinyl]- (CA INDEX NAME)



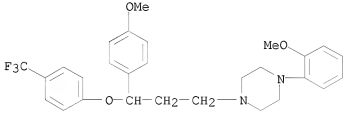
RN 328248-24-4 CAPLUS
CN Piperazine, 1-(2-chlorophenyl)-4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]- (CA INDEX NAME)



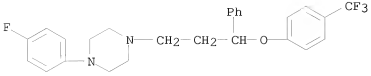
RN 328248-30-2 CAPLUS
CN Piperazine, 1-(4-nitrophenyl)-4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]- (CA INDEX NAME)



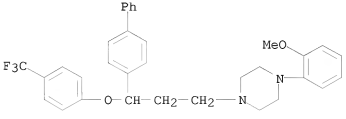
RN 328248-36-8 CAPLUS
CN Piperazine, 1-(2-methoxyphenyl)-4-[3-(4-methoxyphenyl)-3-[4-(trifluoromethyl)phenoxy]propyl]- (CA INDEX NAME)



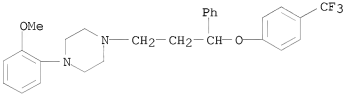
RN 753439-74-6 CAPLUS
CN Piperazine, 1-(4-fluorophenyl)-4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]- (CA INDEX NAME)



RN 767277-20-3 CAPLUS
CN Piperazine, 1-[3-[1,1'-biphenyl]-4-yl-3-[4-(trifluoromethyl)phenoxy]propyl]-4-(2-methoxyphenyl)- (CA INDEX NAME)



RN 777843-82-0 CAPLUS
CN Piperazine, 1-(2-methoxyphenyl)-4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]- (CA INDEX NAME)



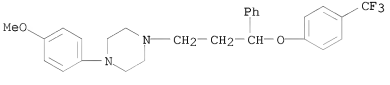
REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 3 OF 16 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2008:232006 CAPLUS
DOCUMENT NUMBER: 148:440268
TITLE: A chemometric study of the 5-HT1A receptor affinities presented by arylpiperazine compounds
AUTHOR(S): Weber, Karen C.; da Silva, Alberico B. F.
CORPORATE SOURCE: Instituto de Quimica de Sao Carlos, Universidade de Sao Paulo, Sao Carlos, 13566-590, Brazil
SOURCE: European Journal of Medicinal Chemistry (2008), 43(2), 364-372
CODEN: EJMCA5; ISSN: 0223-5234
PUBLISHER: Elsevier Masson SAS
DOCUMENT TYPE: Journal
LANGUAGE: English

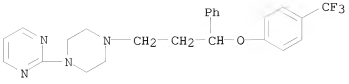
AB Arylpiperazine compds. are promising 5-HT1A receptor ligands that can contribute for accelerating the onset of therapeutic effect of selective serotonin reuptake inhibitors. In the present work, the chemometric methods HCA, PCA, KNN, SIMCA and PLS were employed in order to obtain SAR and QSAR models relating the structures of arylpiperazine compds. to their 5-HT1A receptor affinities. A training set of 52 compds. was used to construct the models and the best ones were obtained with nine topol. descriptors. The classification and regression models were externally validated by means of predictions for a test set of 14 compds. and have presented good quality, as verified by the correctness of classifications, in the case of pattern recognition studies, and by the high correlation coeffs. (q2 = 0.76, r2 = 0.83) and small prediction errors for the PLS regression. Since the results are in good agreement with previous SAR studies, we can suggest that these findings can help in the search for 5-HT1A receptor ligands that are able to improve antidepressant treatment.

IT 328248-21-1 328248-23-3 328248-24-4
328248-30-2 328248-36-8 753439-74-6
767277-20-3 777843-82-0
RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(chemometric study of 5-HT1A receptor affinities presented by arylpiperazine compds. as possible antidepressants)

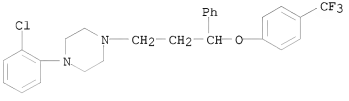
RN 328248-21-1 CAPLUS
CN Piperazine, 1-(4-methoxyphenyl)-4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]- (CA INDEX NAME)



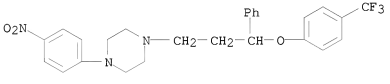
RN 328248-23-3 CAPLUS
CN Pyrimidine, 2-[4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]-1-piperazinyl]- (CA INDEX NAME)



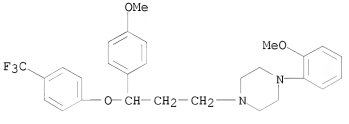
RN 328248-24-4 CAPLUS
CN Piperazine, 1-(2-chlorophenyl)-4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]- (CA INDEX NAME)



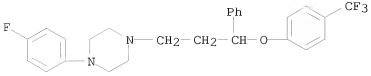
RN 328248-30-2 CAPLUS
CN Piperazine, 1-(4-nitrophenyl)-4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]- (CA INDEX NAME)



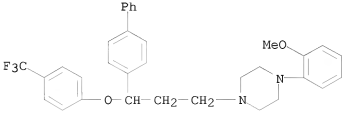
RN 328248-36-8 CAPLUS
CN Piperazine, 1-(2-methoxyphenyl)-4-[3-(4-methoxyphenyl)-3-[4-(trifluoromethyl)phenoxy]propyl]- (CA INDEX NAME)



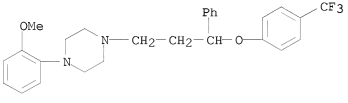
RN 753439-74-6 CAPLUS
CN Piperazine, 1-(4-fluorophenyl)-4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]- (CA INDEX NAME)



RN 767277-20-3 CAPLUS
CN Piperazine, 1-[3-[1,1'-biphenyl]-4-yl-3-[4-(trifluoromethyl)phenoxy]propyl]-4-(2-methoxyphenyl)- (CA INDEX NAME)

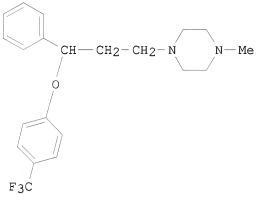


RN 777843-82-0 CAPLUS
CN Piperazine, 1-(2-methoxyphenyl)-4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]- (CA INDEX NAME)



REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 4 OF 16 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2006:847178 CAPLUS
DOCUMENT NUMBER: 145:410017
TITLE: Synthesis of benzenepropanamine analogues as non-detergent spermicides with antitrichomonas and anticandida activities
AUTHOR(S): Kumar, S. T. V. S. Kiran; Sharma, Vishnu Lal; Kumar, Manish; Shukla, Praveen Kumar; Tiwari, Pratibha; Jain, Rajeev Kumar; Maikhuri, Jagdamba Prasad; Singh, Divya; Gupta, Gopal; Singh, Man Mohan
CORPORATE SOURCE: Division of Medicinal and Process Chemistry, Central Drug Research Institute, Lucknow, 226001, India
SOURCE: Bioorganic & Medicinal Chemistry (2006), 14(19), 6593-6600
CODEN: BMECEP; ISSN: 0968-0896
PUBLISHER: Elsevier Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 145:410017
GI

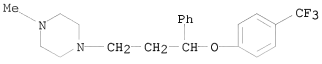


I

AB Fifteen analogs of benzenepropanamine were synthesized and evaluated for their spermicidal as well as microbicidal activities against Trichomonas vaginalis and Candida spp. Several compds. showed appreciable dual activities. Compound I exhibited good spermicidal (MEC = 0.1%) along with substantial anticandidal (MIC = 0.05%) activities, while compds. 3 and 6 showed significant microbicidal activities with moderate spermicidal effect. The SAR of these structures is being discussed here in this communication. It is concluded that suitable structural modifications in this class of compds. at 3-amino position may lead to a potent spermicide with associated microbicidal activity.
IT 911811-07-9P 911811-08-0P 911811-09-1P
911811-11-5P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

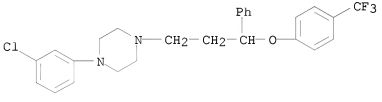
(Uses)
(benzenepropanamine analogs as non-detergent spermicides with antitrichomonas and anticandida activities)

RN 911811-07-9 CAPLUS
CN Piperazine, 1-methyl-4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]-, hydrochloride (1:2) (CA INDEX NAME)



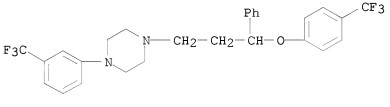
● 2 HCl

RN 911811-08-0 CAPLUS
CN Piperazine, 1-(3-chlorophenyl)-4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

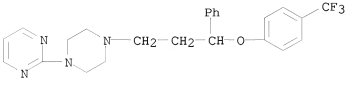
RN 911811-09-1 CAPLUS
CN Piperazine, 1-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]-4-[3-(trifluoromethyl)phenyl]-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

RN 911811-11-5 CAPLUS
CN Pyrimidine, 2-[4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]-1-

piperazinyl]-, hydrochloride (1:2) (CA INDEX NAME)



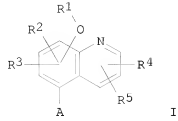
●2 HCl

REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

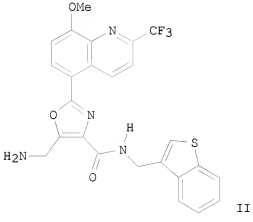
L13 ANSWER 5 OF 16 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2005:1289687 CAPLUS
DOCUMENT NUMBER: 144:51568
TITLE: Preparation of substituted 2-quinolyl-oxazoles and their heterocyclic analogs useful as pde4 inhibitors
INVENTOR(S): Kuang, Rongze; Blythin, David; Shih, Neng-Yang; Shue, Ho-Jane; Chen, Xiao; Cao, Jianhua; Gu, Danlin; Huang, Ying; Schwerdt, John H.; Ting, Pauline C.; Wong, Shing-Chun; Xiao, Li
PATENT ASSIGNEE(S): Schering Corporation, USA
SOURCE: PCT Int. Appl., 233 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005116009	A1	20051208	WO 2005-US17134	20050516
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2005247906	A1	20051208	AU 2005-247906	20050516
CA 2565599	A1	20051208	CA 2005-2565599	20050516
US 20060106062	A1	20060518	US 2005-130359	20050516
EP 1758883	A1	20070307	EP 2005-750076	20050516
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, AL, BA, HR, LV, MK, YU				
CN 1984901	A	20070620	CN 2005-80023666	20050516
BR 2005011295	A	20071204	BR 2005-11295	20050516
JP 2007537300	T	20071220	JP 2007-513471	20050516
TW 286475	B	20070911	TW 2005-94115924	20050517
MX 2006013414	A	20070123	MX 2006-13414	20061117
KR 2007013306	A	20070130	KR 2006-724186	20061117
IN 2006CN04254	A	20070629	IN 2006-CN4254	20061117
NO 2006005830	A	20070216	NO 2006-5830	20061215
PRIORITY APPLN. INFO.:			US 2004-572266P P	20040518
			WO 2005-US17134 W	20050516

OTHER SOURCE(S): CASREACT 144:51568; MARPAT 144:51568
GI



I



II

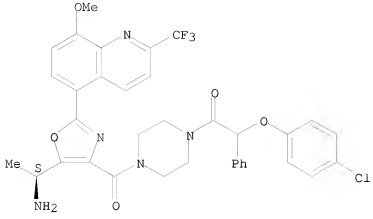
AB Title compds. I [R1 = H, alkyl, cycloalkyl; R2, R3 and R5 independently = H or halo; R4 = H, halo, alkyl, etc.; A = substituted oxazolyl, imidazole, thiazole or pyrrole], and their pharmaceutically acceptable salts, are prepared and disclosed as pde4 inhibitors. Thus, e.g., II was prepared in a multistep synthesis from 2-trifluoromethyl-8-methoxyquinolin-5-yl carboxylic acid. In PDE4 assays, selected compds. possessed IC50 values ranging from 0.01-1.8 nM. Also claimed are pharmaceutical compns., the use of the compds. as PDE4 inhibitors, and combinations with other actives.

IT 871009-78-8P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of substituted quinolyloxazoles and their heterocyclic analogs useful as PDE4 inhibitors)

RN 871009-78-8 CAPLUS

CN Ethanone, 1-[4-[[5-[(1S)-1-aminoethyl]-2-[8-methoxy-2-(trifluoromethyl)-5-quinolinyl]-4-oxazolyl]carbonyl]-1-piperazinyl]-2-(4-chlorophenoxy)-2-phenyl-, hydrochloride (1:1) (CA INDEX NAME)

Absolute stereochemistry.



● HCl

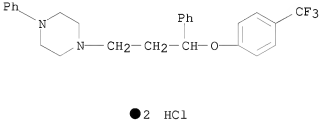
REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 6 OF 16 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2005:1143268 CAPLUS
DOCUMENT NUMBER: 144:63874
TITLE: Design and synthesis of long-chain arylpiperazines with mixed affinity for serotonin transporter (SERT) and 5-HT1A receptor
AUTHOR(S): Perrone, Roberto; Berardi, Francesco; Colabufo, Nicola A.; Lacivita, Enza; Larizza, Carmela; Leopoldo, Marcello; Tortorella, Vincenzo
CORPORATE SOURCE: Dipartimento Farmaco-Chimico, Universita degli Studi di Bari, Bari, 70125, Italy
SOURCE: Journal of Pharmacy and Pharmacology (2005), 57(10), 1319-1327
CODEN: JPPMAB; ISSN: 0022-3573
PUBLISHER: Pharmaceutical Press
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 144:63874

AB A new generation of antidepressant agents could be represented by compds. with mixed activity as serotonin transporter (SERT) inhibitors and 5-HT1A receptor antagonists. We report here on the synthesis and evaluation of SERT and 5-HT1A receptor affinity of long-chain arylpiperazines obtained either by modifying 6-nitroquipazine into a long-chain arylpiperazine or by inserting a modified 6-nitroquipazine moiety or other structures endowed with SERT affinity into a long-chain arylpiperazine with 5-HT1A affinity. Among the compds. studied, 2-[4-(2-methoxyphenyl)piperazin-1-yl]-N-(6-nitro-2-quinolyl)ethylamine (21) and 1-(5-bromo-1,2,3,4-tetrahydronaphthalen-1-yl)-3-[4-(2-methoxyphenyl)-piperazin-1-yl]-1-propanone (24) showed good affinity values for SERT and 5-HT1A receptors (SERT: Ki (inhibition constant) = 71.8 and 62.8 nM; 5-HT1A Ki = 14.2 and 0.82 nM, resp.).

IT 871739-17-2P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(arylpiperazines with mixed affinity for serotonin transporter and 5-HT1A receptor)

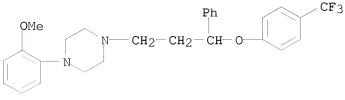
RN 871739-17-2 CAPLUS
CN Piperazine, 1-phenyl-4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]-, hydrochloride (1:2) (CA INDEX NAME)



●2 HCl

IT 777843-82-0
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(arylpiperazines with mixed affinity for serotonin transporter and

5-HT1A receptor)
RN 777843-82-0 CAPLUS
CN Piperazine, 1-(2-methoxyphenyl)-4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]- (CA INDEX NAME)

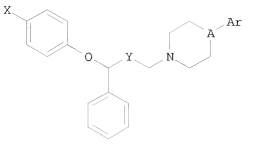


REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

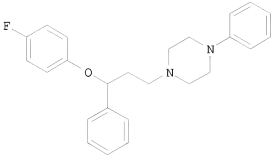
L13 ANSWER 7 OF 16 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2005:1103625 CAPLUS
DOCUMENT NUMBER: 143:387060
TITLE: Preparation of piperazine or piperidine derivatives as serotonin reuptake inhibitors
INVENTOR(S): Pinney, Kevin G.; Miranda, Maria Graciela; Dorsey, James Michael
PATENT ASSIGNEE(S): Baylor University, USA
SOURCE: PCT Int. Appl., 52 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005094896	A2	20051013	WO 2005-US10356	20050328
WO 2005094896	A3	20070503		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, AP, EA, EP, OA				
EP 1732610	A2	20061220	EP 2005-730778	20050328
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, AL, BA, HR, LV, MK, YU				
US 20080132514	A1	20080605	US 2007-594105	20070921
PRIORITY APPLN. INFO.:			US 2004-557069P P	20040326
			WO 2005-US10356 W	20050328

OTHER SOURCE(S): CASREACT 143:387060; MARPAT 143:387060
GI



I



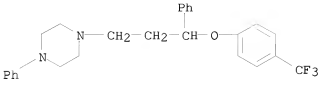
II

AB Title compds. I [X = F or CF3; Y = (CH2)n; n = 0-1; A = N or C; Ar = aryl] and their pharmaceutically acceptable salts, are prepared and disclosed as serotonin reuptake inhibitors. Thus, e.g., II was prepared by reduction of 1-phenyl-3-(4-phenyl-piperazin-1-yl)-propan-1-ol (preparation given) using sodium borohydride followed by coupling with 4-fluorophenol. The ability of I to inhibit [3H]5-HT uptake was evaluated using liquid scintillation spectroscopy and it was revealed that selected compds. of the invention possessed IC50 values in the range of 1.45 up to 9.56 μM. I as serotonin reuptake inhibitors should prove useful in the treatment of depression. Pharmaceutical composition comprising I are disclosed.

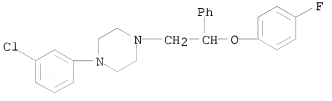
IT 158545-85-8P 691872-56-7P 691872-58-9P
691872-60-3P 691872-62-5P 691872-64-7P
691872-66-9P 866548-21-2P 866548-22-3P
866548-23-4P 866548-24-5P 866548-25-6P
866548-26-7P 866548-27-8P 866548-28-9P
866548-29-0P 866548-30-3P 866548-31-4P
866548-32-5P 866548-33-6P 866548-34-7P
866548-35-8P 866548-36-9P 866548-37-0P
866548-38-1P 866548-39-2P 866548-40-5P
866548-41-6P 866548-42-7P 866548-43-8P
866548-44-9P 866548-45-0P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of piperazine or piperidine derivs. as serotonin reuptake inhibitors)

RN 158545-85-8 CAPLUS

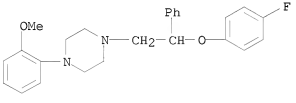
CN Piperazine, 1-phenyl-4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]- (CA INDEX NAME)



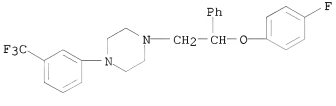
RN 691872-56-7 CAPLUS
CN Piperazine, 1-(3-chlorophenyl)-4-[2-(4-fluorophenoxy)-2-phenylethyl]- (CA INDEX NAME)



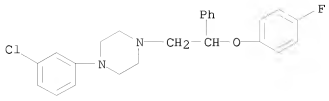
RN 691872-58-9 CAPLUS
CN Piperazine, 1-[2-(4-fluorophenoxy)-2-phenylethyl]-4-(2-methoxyphenyl)- (CA INDEX NAME)



RN 691872-60-3 CAPLUS
CN Piperazine, 1-[2-(4-fluorophenoxy)-2-phenylethyl]-4-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)

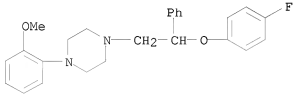


RN 691872-62-5 CAPLUS
CN Piperazine, 1-(3-chlorophenyl)-4-[2-(4-fluorophenoxy)-2-phenylethyl]-, hydrochloride (1:1) (CA INDEX NAME)



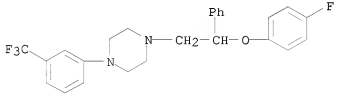
● HCl

RN 691872-64-7 CAPLUS
CN Piperazine, 1-[2-(4-fluorophenoxy)-2-phenylethyl]-4-(2-methoxyphenyl)-, hydrochloride (1:1) (CA INDEX NAME)



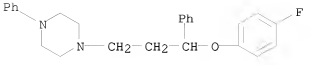
● HCl

RN 691872-66-9 CAPLUS
CN Piperazine, 1-[2-(4-fluorophenoxy)-2-phenylethyl]-4-[3-(trifluoromethyl)phenyl]-, hydrochloride (1:1) (CA INDEX NAME)

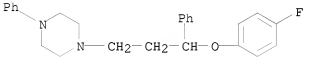


● HCl

RN 866548-21-2 CAPLUS
CN Piperazine, 1-[3-(4-fluorophenoxy)-3-phenylpropyl]-4-phenyl- (CA INDEX NAME)

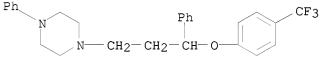


RN 866548-22-3 CAPLUS
CN Piperazine, 1-[3-(4-fluorophenoxy)-3-phenylpropyl]-4-phenyl-, hydrochloride (1:1) (CA INDEX NAME)



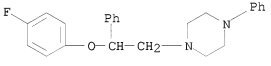
● HCl

RN 866548-23-4 CAPLUS
CN Piperazine, 1-phenyl-4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]-, hydrochloride (1:1) (CA INDEX NAME)

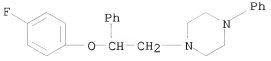


● HCl

RN 866548-24-5 CAPLUS
CN Piperazine, 1-[2-(4-fluorophenoxy)-2-phenylethyl]-4-phenyl- (CA INDEX NAME)

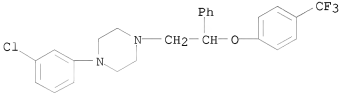


RN 866548-25-6 CAPLUS
CN Piperazine, 1-[2-(4-fluorophenoxy)-2-phenylethyl]-4-phenyl-, hydrochloride (1:1) (CA INDEX NAME)

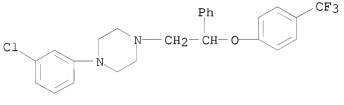


● HCl

RN 866548-26-7 CAPLUS
CN Piperazine, 1-(3-chlorophenyl)-4-[2-phenyl-2-[4-(trifluoromethyl)phenoxy]ethyl]- (CA INDEX NAME)

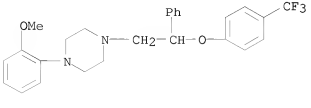


RN 866548-27-8 CAPLUS
CN Piperazine, 1-(3-chlorophenyl)-4-[2-phenyl-2-[4-(trifluoromethyl)phenoxy]ethyl]-, hydrochloride (1:1) (CA INDEX NAME)

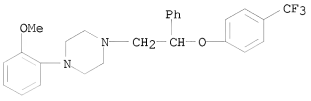


● HCl

RN 866548-28-9 CAPLUS
CN Piperazine, 1-(2-methoxyphenyl)-4-[2-phenyl-2-[4-(trifluoromethyl)phenoxy]ethyl]- (CA INDEX NAME)

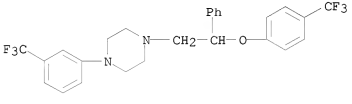


RN 866548-29-0 CAPLUS
CN Piperazine, 1-(2-methoxyphenyl)-4-[2-phenyl-2-[4-(trifluoromethyl)phenoxy]ethyl]-, hydrochloride (1:1) (CA INDEX NAME)

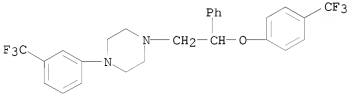


● HCl

RN 866548-30-3 CAPLUS
CN Piperazine, 1-[2-phenyl-2-[4-(trifluoromethyl)phenoxy]ethyl]-4-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)

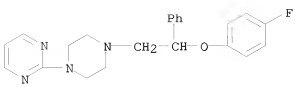


RN 866548-31-4 CAPLUS
CN Piperazine, 1-[2-phenyl-2-[4-(trifluoromethyl)phenoxy]ethyl]-4-[3-(trifluoromethyl)phenyl]-, hydrochloride (1:1) (CA INDEX NAME)

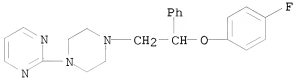


● HCl

RN 866548-32-5 CAPLUS
CN Pyrimidine, 2-[4-[2-(4-fluorophenoxy)-2-phenylethyl]-1-piperazinyl]- (CA INDEX NAME)

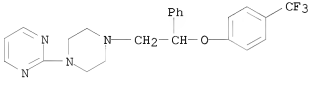


RN 866548-33-6 CAPLUS
CN Pyrimidine, 2-[4-[2-(4-fluorophenoxy)-2-phenylethyl]-1-piperazinyl]-, hydrochloride (1:1) (CA INDEX NAME)

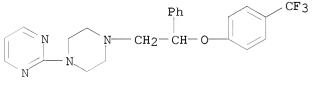


● HCl

RN 866548-34-7 CAPLUS
CN Pyrimidine, 2-[4-[2-phenyl-2-[4-(trifluoromethyl)phenoxy]ethyl]-1-piperazinyl]- (CA INDEX NAME)



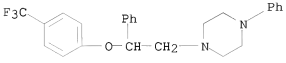
RN 866548-35-8 CAPLUS
CN Pyrimidine, 2-[4-[2-phenyl-2-[4-(trifluoromethyl)phenoxy]ethyl]-1-piperazinyl]-, hydrochloride (1:1) (CA INDEX NAME)



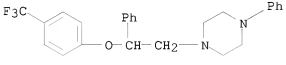
● HCl

RN 866548-36-9 CAPLUS

CN Piperazine, 1-phenyl-4-[2-phenyl-2-[4-(trifluoromethyl)phenoxy]ethyl]- (CA INDEX NAME)

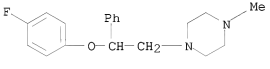


RN 866548-37-0 CAPLUS
CN Piperazine, 1-phenyl-4-[2-phenyl-2-[4-(trifluoromethyl)phenoxy]ethyl]-, hydrochloride (1:1) (CA INDEX NAME)

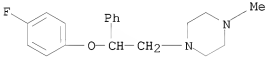


● HCl

RN 866548-38-1 CAPLUS
CN Piperazine, 1-[2-(4-fluorophenoxy)-2-phenylethyl]-4-methyl- (CA INDEX NAME)

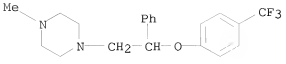


RN 866548-39-2 CAPLUS
CN Piperazine, 1-[2-(4-fluorophenoxy)-2-phenylethyl]-4-methyl-, hydrochloride (1:1) (CA INDEX NAME)

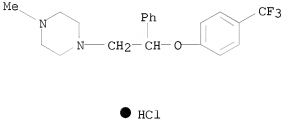


● HCl

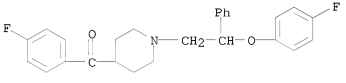
RN 866548-40-5 CAPLUS
CN Piperazine, 1-methyl-4-[2-phenyl-2-[4-(trifluoromethyl)phenoxy]ethyl]- (CA INDEX NAME)



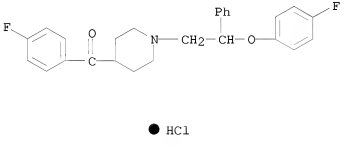
RN 866548-41-6 CAPLUS
CN Piperazine, 1-methyl-4-[2-phenyl-2-[4-(trifluoromethyl)phenoxy]ethyl]-, hydrochloride (1:1) (CA INDEX NAME)



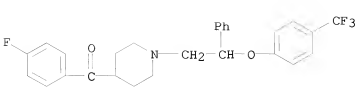
RN 866548-42-7 CAPLUS
CN Methanone, [1-[2-(4-fluorophenoxy)-2-phenylethyl]-4-piperidinyl](4-fluorophenyl)- (CA INDEX NAME)



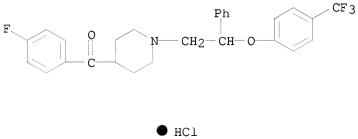
RN 866548-43-8 CAPLUS
CN Methanone, [1-[2-(4-fluorophenoxy)-2-phenylethyl]-4-piperidinyl](4-fluorophenyl)-, hydrochloride (1:1) (CA INDEX NAME)



RN 866548-44-9 CAPLUS
CN Methanone, (4-fluorophenyl)[1-[2-phenyl-2-[4-(trifluoromethyl)phenoxy]ethyl]-4-piperidinyl]- (CA INDEX NAME)



RN 866548-45-0 CAPLUS
CN Methanone, (4-fluorophenyl)[1-[2-phenyl-2-[4-(trifluoromethyl)phenoxy]ethyl]-4-piperidinyl]-, hydrochloride (1:1) (CA INDEX NAME)

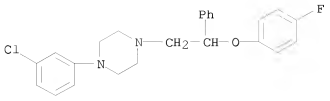


L13 ANSWER 8 OF 16 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2004:170822 CAPLUS
DOCUMENT NUMBER: 140:417233
TITLE: Synthesis and biological evaluation of 2-(4-fluorophenoxy)-2-phenyl-ethyl piperazines as serotonin-selective reuptake inhibitors with a potentially improved adverse reaction profile
AUTHOR(S): Dorsey, James M.; Miranda, Maria G.; Cozzi, Nicholas V.; Pinney, Kevin G.
CORPORATE SOURCE: Department of Chemistry and Biochemistry and The Center for Drug Discovery, Baylor University, Waco, TX, 76798-7348, USA
SOURCE: Bioorganic & Medicinal Chemistry (2004), 12(6), 1483-1491
CODEN: BMECEP; ISSN: 0968-0896
PUBLISHER: Elsevier Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 140:417233

AB Three new 2-(4-fluorophenoxy)-2-phenyl-Et piperazines, 1-(3-chlorophenyl)-4-[2-(4-fluorophenoxy)-2-phenylethyl]-piperazine, 1-[2-(4-fluorophenoxy)-2-phenylethyl]-4-(2-methoxyphenyl)-piperazine, and 1-[2-(4-fluorophenoxy)-2-phenylethyl]-4-(3-trifluoromethylphenyl)-piperazine, modeled after the potent antidepressant fluoxetine and coupled with several functionalized piperazines, have been prepared by chemical synthesis as selective serotonin reuptake inhibitors (SSRIs) with a potentially improved adverse reaction profile. Typical SSRIs, although very effective in the treatment of depression, still face the troublesome side effect of sexual dysfunction. A number of pharmacol. agents-notably, drugs in the piperazine class-have been used to reverse SSRI-induced sexual dysfunction, and evidence for developing an improved SSRI by coupling a fluoxetine congener with the pharmacophore of a reversal agent holds promise. Preliminary data indicates that the hydrochloride (HCl) salts of piperazines exhibit single-site binding at the site of the serotonin reuptake transporter (SERT). However, each of the three compds. are much less potent than typical SSRIs, showing micromolar (μM) affinity for the SERT with IC50 values of 1.45 μM, 3.27 μM, and 9.56 μM, resp. Further biol. evaluation of piperazine compds. is needed before definitive conclusions can be made with regard to each compound's potential for use as an SSRI-type candidate which is devoid of sexual side effects. Nevertheless, the initial findings are quite encouraging, thus lending credence to the idea of hybridizing an SSRI congener with that of the pharmacophore of an agent known to reverse or treat SSRI-induced sexual dysfunction.

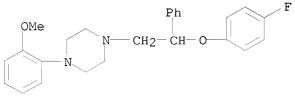
IT 691872-62-5P 691872-64-7P 691872-66-9P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(synthesis and structure-activity relationship of 2-(4-fluorophenoxy)-2-Ph-Et piperazines as serotonin-selective reuptake inhibitors with a potentially improved adverse reaction profile)

RN 691872-62-5 CAPLUS
CN Piperazine, 1-(3-chlorophenyl)-4-[2-(4-fluorophenoxy)-2-phenylethyl]-, hydrochloride (1:1) (CA INDEX NAME)



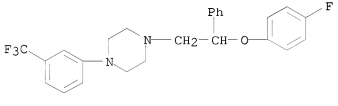
● HCl

RN 691872-64-7 CAPLUS
CN Piperazine, 1-[2-(4-fluorophenoxy)-2-phenylethyl]-4-(2-methoxyphenyl)-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

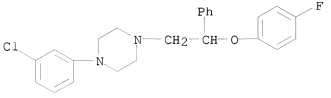
RN 691872-66-9 CAPLUS
CN Piperazine, 1-[2-(4-fluorophenoxy)-2-phenylethyl]-4-[3-(trifluoromethyl)phenyl]-, hydrochloride (1:1) (CA INDEX NAME)



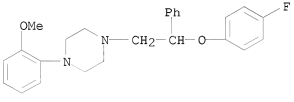
● HCl

IT 691872-56-7P 691872-58-9P 691872-60-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis and structure-activity relationship of 2-(4-fluorophenoxy)-2-Ph-Et piperazines as serotonin-selective reuptake inhibitors with a potentially improved adverse reaction profile)
RN 691872-56-7 CAPLUS

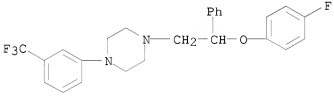
CN Piperazine, 1-(3-chlorophenyl)-4-[2-(4-fluorophenoxy)-2-phenylethyl]- (CA INDEX NAME)



RN 691872-58-9 CAPLUS
CN Piperazine, 1-[2-(4-fluorophenoxy)-2-phenylethyl]-4-(2-methoxyphenyl)- (CA INDEX NAME)

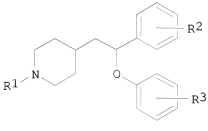


RN 691872-60-3 CAPLUS
CN Piperazine, 1-[2-(4-fluorophenoxy)-2-phenylethyl]-4-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 9 OF 16 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2003:860624 CAPLUS
DOCUMENT NUMBER: 140:76994
TITLE: Syntheses and Binding Studies of New [(Aryl)(aryloxy)methyl]piperidine Derivatives and Related Compounds as Potential Antidepressant Drugs with High Affinity for Serotonin (5-HT) and Norepinephrine (NE) Transporters
AUTHOR(S): Orjales, Aurelio; Mosquera, Ramon; Toledo, Antonio; Pumar, M. Carmen; Garcia, Neftali; Cortizo, Lourdes; Labeaga, Luis; Innerarity, Ana
CORPORATE SOURCE: Research Department, FAES FARMA S. A., Leioa, Vizcaya, 48940, Spain
SOURCE: Journal of Medicinal Chemistry (2003), 46(25), 5512-5532
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 140:76994
GI



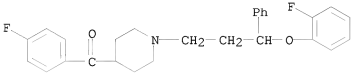
I

AB In a wide search program toward new, efficient, and fast-acting antidepressant drugs, series of new compds. having an (aryl)(aryloxy)methyl moiety linked directly or through a methylene chain to different substituted and unsubstituted cycles (isoquinoline, piperazine, piperidine, tetrahydropyran, or cyclopentane) were prepared These compds. have been evaluated for their affinities for serotonin (5-HT) transporter (SERT) and 5-HT1A and 5-HT2A receptors. Racemic mixts. of 4-[(aryl)(aryloxy)methyl]piperidines I (R1 = H, Me, MeCO; R2 = H, 3-F, 4-F, 4-Cl, 4-Me; R3 = H, 2-CN, 4-O2N, 4-MeO, 2-Ph, etc.) showed much higher affinity values for SERT than fluoxetine and resulted in lack of affinity for 5-HT1A and 5-HT2A receptors. Some of these racemic mixts. were resolved to their enantiomers and tested for binding to norepinephrine (NE) transporter (NET), dopamine (DA) transporter (DAT), and α2 receptor. Several of these enantiomers, (-)-I (R1 = R2 = H; R3 = 2-F), (-)-I (R1 = R2 = H; R3 = 3-F), (-)-I (R1 = H; R2 = 3-F; R3 = 2-F), (+)-I (R1 = H; R2 = R3 = 3-F), displayed a dual binding profile with affinities for SERT and NET with Ki < 25 nM and a NET/SERT ratio <10. (-)-I (R1 = R2 = H; R3 = 3-F) (coded as F-98214-TA for development studies) showed a dual binding profile with very high affinity values for SERT and NET (Ki = 1.9 and 13.5 nM, resp.), and further pharmacol. characterization is in progress for its evaluation as a antidepressant.
IT 639467-63-3P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of [(aryl)(aryloxy)alkyl]piperidines and analogs as potential antidepressants with high affinity for serotonin and norepinephrine transporters)

RN 639467-63-3 CAPLUS

CN Methanone, [1-[3-(2-fluorophenoxy)-3-phenylpropyl]-4-piperidinyl](4-fluorophenyl)-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

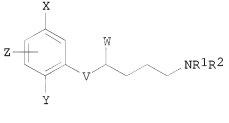
REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 10 OF 16 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2001:636031 CAPLUS
DOCUMENT NUMBER: 135:210828
TITLE: Preparation of novel phenylheteroalkylamines as inhibitors of nitric oxide synthase
INVENTOR(S): Birkinshaw, Tim; Cheshire, David; Mete, Antonio
PATENT ASSIGNEE(S): Astrazeneca AB, Swed.
SOURCE: PCT Int. Appl., 88 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001062713	A1	20010830	WO 2001-SE370	20010220
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
AU 2001034313	A	20010903	AU 2001-34313	20010220
EP 1263714	A1	20021211	EP 2001-906490	20010220
EP 1263714	B1	20040428		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2003523992	T	20030812	JP 2001-561723	20010220
AT 265422	T	20040515	AT 2001-906490	20010220
US 20030105161	A1	20030605	US 2002-204815	20020822
US 6743939	B2	20040601		

PRIORITY APPLN. INFO.: GB 2000-4149 A 20000223
WO 2001-SE370 W 20010220

OTHER SOURCE(S): MARPAT 135:210828
GI



I

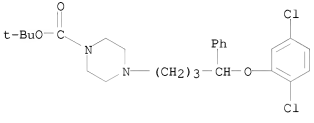
AB The title compds. [I; X, Y = alkyl, alkoxy, halo, etc.; Z = H, F; V = O, SOn, NR3; W = alkyl, alkenyl, Ph, etc.; R1, R2 = H, alkyl, cycloalkyl, etc.; NR1R2 = (un)substituted 4-8 membered saturated azacyclic ring optionally

incorporating one further heteroatom selected from O, S or NR8, 5-membered aromatic azacyclic ring optionally incorporating one further N atom; R3 = H, alkyl; R8 = H, alkyl, etc.; n = 0-2] and their pharmaceutically acceptable salts which are inhibitors of nitric oxide synthase and are thereby particularly useful in the treatment or prophylaxis of inflammatory disease and pain, were prepared E.g., a 4-step synthesis of (1R)-I.oxalate [X = Cl; Y = CN; Z = H; V = O; W = Ph; R1 = H; R2 = Me] was given. The exemplified compds. I (with the exception of one) showed IC50 of < 40 μM against nitric oxide synthase.

IT 357443-66-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of novel phenylheteroalkylamines as inhibitors of nitric oxide synthase)

RN 357443-66-4 CAPLUS

CN 1-Piperazinecarboxylic acid, 4-[4-(2,5-dichlorophenoxy)-4-phenylbutyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)



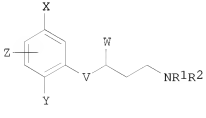
REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 11 OF 16 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2001:636023 CAPLUS
DOCUMENT NUMBER: 135:210827
TITLE: Preparation of phenylheteroalkylamines as inhibitors of nitric oxide synthase
INVENTOR(S): Cheshire, David; Connolly, Stephen; Cox, David; Hamley, Peter; Mete, Antonio; Pimm, Austen
PATENT ASSIGNEE(S): Astrazeneca AB, Swed.
SOURCE: PCT Int. Appl., 135 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001062704	A1	20010830	WO 2001-SE373	20010220
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2397234	A1	20010830	CA 2001-2397234	20010220
BR 2001008613	A	20021112	BR 2001-8613	20010220
EP 1263711	A1	20021211	EP 2001-906492	20010220
EP 1263711	B1	20041215		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2003523988	T	20030812	JP 2001-561714	20010220
AT 284860	T	20050115	AT 2001-906492	20010220
AU 781141	B2	20050505	AU 2001-34315	20010220
CN 1235870	C	20060111	CN 2001-805489	20010220
NZ 520107	A	20060224	NZ 2001-520107	20010220
NO 2002004014	A	20020925	NO 2002-4014	20020822
MX 2002008203	A	20021129	MX 2002-8203	20020822
US 20030158185	A1	20030821	US 2002-204742	20021018
US 6887871	B2	20050503		

PRIORITY APPLN. INFO.:		GB 2000-4153	A 20000223
		WO 2001-SE373	W 20010220

OTHER SOURCE(S): MARPAT 135:210827
GI



I

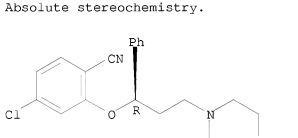
AB The title compds. [I; X, Y = alkyl, alkoxy, halo, etc.; Z = H, F; V = O; W = (un)substituted Ph, 5-6 membered aromatic heterocyclic ring containing 1-3 heteroatoms selected from O, S and N; R1, R2 = H, alkyl, cycloalkyl, etc.; or NR1R2 = (un)substituted 4-8 membered saturated azacyclic ring optionally incorporating one further heteroatom selected from O, S or NR8, 5-membered aromatic azacyclic ring optionally incorporating one further N atom; R8 = H, alkyl, etc.] and their pharmaceutically acceptable salts which are inhibitors of the enzyme nitric oxide synthase and are thereby particularly useful in the treatment or prophylaxis of inflammatory disease, were prepared Thus, protecting α-(2-aminoethyl)benzenemethanol with di-tert-Bu dicarbonate followed by reacting the resulting carbamate with 4-chloro-2-hydroxybenzonitrile in the presence of triphenylphosphine and di-Et diazodicarboxylate in PhMe/THF, and deprotection of the amine afforded I.HCl [X = Cl; Y = CN, Z = H; V = O; W = Ph; R1, R2 = H]. The exemplified compds. I showed IC50 of < 25 μM against nitric oxide synthase.

IT 357401-87-7P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of phenylheteroalkylamines as inhibitors of nitric oxide synthase)

RN 357401-87-7 CAPLUS

CN Benzonitrile, 4-chloro-2-[(1R)-3-(4-methyl-1-piperazinyl)-1-phenylpropoxy]-, hydrochloride (1:2) (CA INDEX NAME)

Absolute stereochemistry.



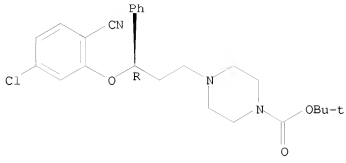
●2 HCl

IT 357405-84-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of phenylheteroalkylamines as inhibitors of nitric oxide synthase)

RN 357405-84-6 CAPLUS

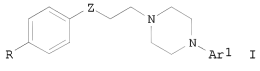
CN 1-Piperazinecarboxylic acid, 4-[(3R)-3-(5-chloro-2-cyanophenoxy)-3-phenylpropyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

Absolute stereochemistry.

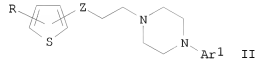


REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

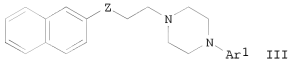
L13 ANSWER 12 OF 16 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2001:76 CAPLUS
DOCUMENT NUMBER: 134:207795
TITLE: New 1-aryl-3-(4-arylpiperazin-1-yl)propane derivatives, with dual action at 5-HT1A serotonin receptors and serotonin transporter, as a new class of antidepressants
AUTHOR(S): Martinez-Esparza, Javier; Oficialdegui, Ana-M.; Perez-Silanes, Silvia; Heras, Begona; Orus, Lara; Palop, Juan-A.; Lasheras, Berta; Roca, Joan; Mourelle, Marisa; Bosch, Ana; Del Castillo, Juan-C.; Tordera, Rosa; Del Rio, Joaquin; Monge, Antonio
CORPORATE SOURCE: Departments of Medicinal Chemistry and Pharmacology Centro de Investigacion en Farmacobiologia Aplicada (CIFA), Universidad de Navarra, Pamplona, 31080, Spain
SOURCE: Journal of Medicinal Chemistry (2001), 44(3), 418-428 CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 134:207795
GI



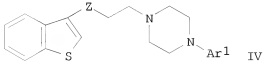
I



II



III



IV

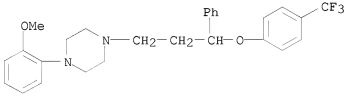
AB In a search toward new and efficient antidepressants, 1-aryl-3-(4-arylpiperazin-1-yl)propane derivs. I (R = H, Ph, MeO, NO2, Z = CO, CHOH, CHOR1, R1 = 4-F3CC6H4, 4-MeOC6H4, 3,4-OCH3OC6H3, Ar1 =

2-MeOC6H4, 4-ClC6H4, 2-pyridyl, etc.), II (R = H, 2,5-Me2, 5-Me, 5-NO2, Z = CO, CNOH, CHOH, CHOR1, R1 = 4-F3CC6H4, 3,4-OCH2OC6H3, 1-C10H7, position = 2, 3), III and IV (Ar1 = 2-MeOC6H4, 4-ClC6H4, 2-HOC6H4, Z = CO,CHOH) were designed, synthesized, and evaluated for 5-HT reuptake inhibition and 5-HT1A receptor antagonism. This dual pharmacol. profile should lead, in principle, to a rapid and pronounced enhancement in serotoninergic neurotransmission and consequently to a more efficacious treatment of depression. The design was based on coupling structural moieties related to inhibition of serotonin reuptake, such as γ-phenoxypropylamines, to arylpiperazines, typical 5-HT1A ligands. In binding studies, several compds. showed affinity at the 5-HT transporter and 5-HT1A receptors. Antidepressant-like activity was initially assayed in the forced swimming test with those compds. with Ki < 200 nM in both binding studies. Functional characterization was performed by measuring the intrinsic effect on rectal temperature in mice and also the antagonism to 8-OH-DPAT-induced hypothermia. The most efficacious compds. II (R = H, Z = CHO-1-C10H7, position = 3, Ar1 = 2-MeOC6H4) (V), II[R = 5-Me, Z = (E)-CNOH, position = 2, Ar1 = 2-MeOC6H4] and IV (Z = CO, CHOH, Ar1 = 2-MeOC6H4) (VI) were further explored for their ability to antagonize 8-OH-DPAT-induced inhibition of forskolin-stimulated cAMP formation in a cell line expressing the 5-HT1A receptor. Furthermore, the antidepressant-like properties of V and VI, which exhibited 5-HT1A receptor antagonistic property in the latter study, were also evaluated in the learned helplessness test in rats. Among these three compds., VI (Z = CHOH) (1-benzo[b]thiophene-3-yl)-3-[4-(2-methoxyphenyl)-1-yl]propan-1-ol] showed the higher affinity at both the 5-HT transporter and 5-HT1A receptors (Ki = 20 nM in both cases) and was also active in the other pharmacol. tests. Such a pharmacol. profile could lead to a new class of antidepressants with a dual mechanism of action and a faster onset of action.

IT 328248-11-9P 328248-15-3P 328248-21-1P
328248-23-3P 328248-24-4P 328248-26-6P
328248-30-2P 328248-33-5P 328248-36-8P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation, 5-HT1A serotonin receptor antagonist and serotonin transporter activity, and structure-activity relationship of aryl(arylpiperazinyl)propanes)

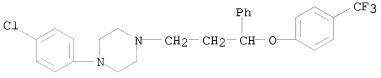
RN 328248-11-9 CAPLUS

CN Piperazine, 1-(2-methoxyphenyl)-4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]-, hydrochloride (1:2) (CA INDEX NAME)

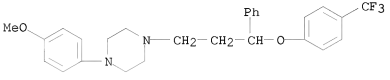


●2 HCl

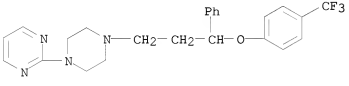
RN 328248-15-3 CAPLUS
CN Piperazine, 1-(4-chlorophenyl)-4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]- (CA INDEX NAME)



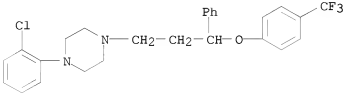
RN 328248-21-1 CAPLUS
CN Piperazine, 1-(4-methoxyphenyl)-4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]- (CA INDEX NAME)



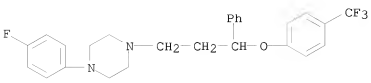
RN 328248-23-3 CAPLUS
CN Pyrimidine, 2-[4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]-1-piperazinyl]- (CA INDEX NAME)



RN 328248-24-4 CAPLUS
CN Piperazine, 1-(2-chlorophenyl)-4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]- (CA INDEX NAME)

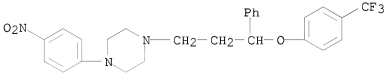


RN 328248-26-6 CAPLUS
CN Piperazine, 1-(4-fluorophenyl)-4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]-, hydrochloride (1:2) (CA INDEX NAME)

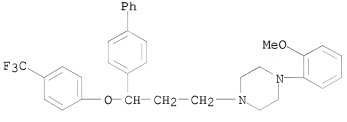


●2 HCl

RN 328248-30-2 CAPLUS
CN Piperazine, 1-(4-nitrophenyl)-4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]- (CA INDEX NAME)

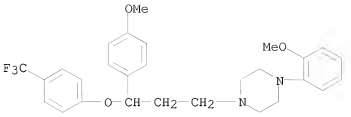


RN 328248-33-5 CAPLUS
CN Piperazine, 1-[3-[1,1'-biphenyl]-4-yl-3-[4-(trifluoromethyl)phenoxy]propyl]-4-(2-methoxyphenyl)-, hydrochloride (1:2) (CA INDEX NAME)



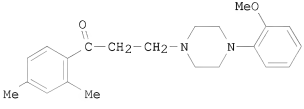
●2 HCl

RN 328248-36-8 CAPLUS
CN Piperazine, 1-(2-methoxyphenyl)-4-[3-(4-methoxyphenyl)-3-[4-(trifluoromethyl)phenoxy]propyl]- (CA INDEX NAME)



REFERENCE COUNT: 54 THERE ARE 54 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 13 OF 16 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2000:601312 CAPLUS
DOCUMENT NUMBER: 133:305272
TITLE: Design, synthesis and biological evaluation of new 3-[(4-aryl)piperazin-1-yl]-1-arylpropane derivatives as potential antidepressants with a dual mode of action; serotonin reuptake inhibition and 5-HT1A receptor antagonism
AUTHOR(S): Oficialdegui, A. M.; Martinez, J.; Perez, S.; Heras, B.; Irurzun, M.; Palop, J. A.; Tordera, R.; Lasheras, B.; Del Rio, J.; Monge, A.
CORPORATE SOURCE: Department of Medicinal Chemistry, Centro de Investigacion en Farmacobiologia Aplicada (CIFA), Universidad de Navarra, Pamplona, 31080, Spain
SOURCE: Farmaco (2000), 55(5), 345-353
CODEN: FRMCE8; ISSN: 0014-827X
PUBLISHER: Elsevier Science S.A.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 133:305272
GI

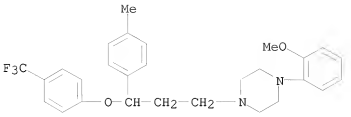


I

AB It has been suggested that the combination of a selective serotonin reuptake inhibitor (SSRI) and a 5-HT1A receptor antagonist may facilitate the onset of the SSRIs antidepressant action. Accordingly, we describe the synthesis of a series of new 3-[(4-aryl)piperazin-1-yl]-1-arylpropane derivs. with structural modifications performed in Ar1, Ar2 and Z (Z is different functional groups) to obtain the sought dual activity. Compds. were evaluated for in vitro affinity at 5-HT1A receptors and 5-HT transporter. The antidepressant-like activity of derivs. with the higher affinity was assessed initially using the forced swimming test (FST). Compound 1-(2,4-dimethylphenyl)-3-[(2-methoxyphenyl)piperazin-1-yl]-1-propanone (I) showed the best antidepressant-like activity which was further confirmed in the learned helplessness test.

IT 302561-62-2P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(design, synthesis and antidepressant activity of [(aryl)piperazinyl]arylpropane derivs.)

RN 302561-62-2 CAPLUS
CN Piperazine, 1-(2-methoxyphenyl)-4-[3-(4-methylphenyl)-3-[4-(trifluoromethyl)phenoxy]propyl]- (CA INDEX NAME)



REFERENCE COUNT: 42 THERE ARE 42 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 14 OF 16 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1994:655827 CAPLUS
DOCUMENT NUMBER: 121:255827
ORIGINAL REFERENCE NO.: 121:46707a,46710a
TITLE: Preparation of (hetero)arylpropanolamine derivatives as cerebral calcium overload blockers
INVENTOR(S): Jakobsen, Palle; Kanstrup, Anders; Lundbeck, Jane Marie
PATENT ASSIGNEE(S): Novo Nordisk A/S, Den.
SOURCE: Eur. Pat. Appl., 18 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

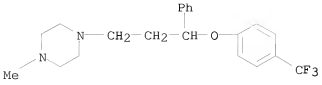
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 576766	A1	19940105	EP 1992-610053	19920629
R: GB				
PRIORITY APPLN. INFO.:			EP 1992-610053	19920629
OTHER SOURCE(S):	MARPAT 121:255827			

AB XR3(RO)CCR4R5CR6R7NR1R2 [X = Ph optionally substituted with one or more cyano, halo, haloalkyl, alkoxy, alkyl, alkanoyl, alkenyl, aryloxy, aralkoxy, amino, alkyl mono or disubstituted amino, alkanoylamino, carbamoyl, alkyl mono- or disubstituted carbamoyl, alkyl substituted with amino, alkyl mono or disubstituted amino, NO2, morpholino, imidazolyl; R = 3,4-methylenedioxyphenyl, aryl or heteroaryl all of which can be optionally substituted with one or more cyano, halogeno, alkyl, alkoxy, alkenyl, trifluoromethyl, alkylene, aryloxy, aralkoxy, alkylthio; R1, R2 = alkyl, cycloalkyl, alkenyl, cycloalkylalkyl, all of which can be unsubstituted or substituted with alkyl, alkoxy or cyano; R1R2 = 5-, 6- or 7-membered ring containing ≥1 N atom, or which optionally contains 2 N atoms, one or 2 O atom(s) or one or 2 S atom(s) or a combination thereof, which ring is optionally substituted with alkyl, alkoxy, or aryl; and R3-R7 = H, alkyl, phenyl; R4X = carbocyclic ring containing 5 or 6 atoms; or salts thereof with a pharmaceutically acceptable acid; with provisos], were prepared Thus, 1-(4-cyanophenyl)-3-piperidinylpropan-1-ol was condensed with 4-trifluoromethylbenzotrifluoride using KOCMe3 to give 1-[3-(4-cyanophenyl)-3-(4-trifluoromethylphenoxy)propyl]piperidine, isolated as the oxalate. The latter inhibited stimulated uptake of 45Ca by rat P2 synaptosomal prepns. with IC50 = 2.2 μg/mL, vs. 26 μg/mL for nifedipine. Generic I formulations are given.

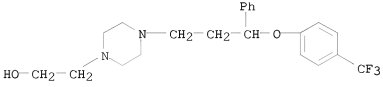
IT 158545-83-6P 158545-84-7P 158545-85-8P
158546-05-5P 158546-06-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as cerebral calcium overload blocker)

RN 158545-83-6 CAPLUS

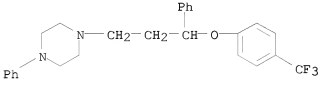
CN Piperazine, 1-methyl-4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]- (CA INDEX NAME)



RN 158545-84-7 CAPLUS
CN 1-Piperazineethanol, 4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]-
(CA INDEX NAME)



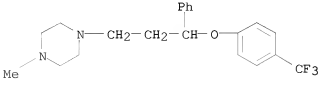
RN 158545-85-8 CAPLUS
CN Piperazine, 1-phenyl-4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]-
(CA INDEX NAME)



RN 158546-05-5 CAPLUS
CN Piperazine, 1-methyl-4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]-,
ethanedioate (1:1) (CA INDEX NAME)

CM 1

CRN 158545-83-6
CMF C21 H25 F3 N2 O



CM 2

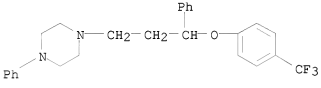
CRN 144-62-7

CMF C2 H2 O4

RN 158546-06-6 CAPLUS
CN Piperazine, 1-phenyl-4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]-, ethanedioate (1:1) (CA INDEX NAME)

CM 1

CRN 158545-85-8
CMF C26 H27 F3 N2 O



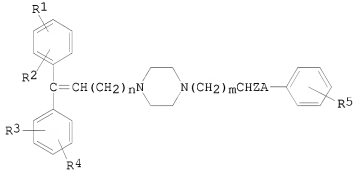
CM 2

CRN 144-62-7
CMF C2 H2 O4

L13 ANSWER 15 OF 16 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1989:95279 CAPLUS
DOCUMENT NUMBER: 110:95279
ORIGINAL REFERENCE NO.: 110:15755a,15758a
TITLE: 1-[(1,1-Diphenyl)-1-alkenyl]piperazine derivatives as antidepressants and their preparation
INVENTOR(S): Buzas, Andre; Ollivier, Roland
PATENT ASSIGNEE(S): Laboratoires Meram, Fr.
SOURCE: Eur. Pat. Appl., 22 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 288360	A1	19881026	EP 1988-400903	19880414
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
FR 2614021	A1	19881021	FR 1987-5311	19870414
FR 2614021	B1	19910301		
FI 8801633	A	19881015	FI 1988-1633	19880408
NO 8801554	A	19881017	NO 1988-1554	19880411
US 4882331	A	19891121	US 1988-179750	19880411
DK 8802009	A	19881015	DK 1988-2009	19880413
JP 63258862	A	19881026	JP 1988-89163	19880413
CA 1295617	C	19920211	CA 1988-564057	19880413
AU 8814634	A	19881020	AU 1988-14634	19880414
AU 605275	B2	19910110		
ZA 8802633	A	19881228	ZA 1988-2633	19880414

PRIORITY APPLN. INFO.: FR 1987-5311 A 19870414
OTHER SOURCE(S): CASREACT 110:95279; MARPAT 110:95279
GI



I

AB The title compds. I [R1-R5 = H, halo, C1-6 alkyl, alkenyl, etc.; n = 1-3; m = 0-3; Z = H, C1-6 alkyl, (substituted) Ph; A = O, CO] and pharmaceutically acceptable salts thereof, useful as antidepressants, were prepared N-Alkylation of 1-(1,1-diphenyl-1-buten-4-yl)piperazine with 2-bromo-1-(4-fluorophenoxy)ethane gave (after treatment with MeSO3H) gave I.2MeSO3H (R1-R4 = H, Z = H, R5 = 4-F, n = 2, m = 1, A = O) (II). II at 18.8 mg/kg i.p. inhibited head twitches induced by 5-hydroxytryptophan in

mice.

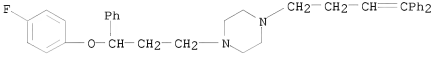
IT 118976-76-4P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, as antidepressant)

RN 118976-76-4 CAPLUS

CN Piperazine, 1-(4,4-diphenyl-3-butenyl)-4-[3-(4-fluorophenoxy)-3-phenylpropyl]-, dimethanesulfonate (9CI) (CA INDEX NAME)

CM 1

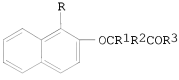
CRN 118976-75-3
CMF C35 H37 F N2 O



CM 2

CRN 75-75-2
CMF C H4 O3 S

L13 ANSWER 16 OF 16 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1979:132586 CAPLUS
DOCUMENT NUMBER: 90:132586
ORIGINAL REFERENCE NO.: 90:20867a,20870a
TITLE: Smooth muscle relaxant properties of 2-naphthyl-oxyacetic acid amides
AUTHOR(S): Pestellini, Vittorio; Ghelardoni, Mario; Del Soldato, Piero; Volterra, Giovanna
CORPORATE SOURCE: Res. Lab., A. Menarini Pharm., Florence, Italy
SOURCE: European Journal of Medicinal Chemistry (1978), 13(5), 486
CODEN: EJMCA5; ISSN: 0009-4374
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

AB Twenty-eight 2-naphthyloxyacetamides (I; R = H or Cl; R1 = H or Me; R2 = H, Me, or Ph; R3 = NHR or 4-substituted piperazinyl) were synthesized by reaction of the appropriate amines with the acylchlorides, and were tested for their smooth muscle relaxant properties in vitro and in vivo. Quaternary salts were prepared by treatment of the tertiary bases with MeBr. Structure-biol. activity relations are discussed.

IT 69478-96-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and smooth muscle-relaxant activity of)

RN 69478-96-2 CAPLUS

CN Ethanone, 2-[(1-chloro-2-naphthalenyl)oxy]-1-(4-methyl-1-piperazinyl)-2-phenyl- (CA INDEX NAME)

```
=> d his

     (FILE 'HOME' ENTERED AT 16:23:34 ON 10 MAR 2009)

     FILE 'REGISTRY' ENTERED AT 16:24:30 ON 10 MAR 2009
L1             STRUCTURE UPLOADED
L2           116 S L1 FULL

     FILE 'CAPLUS' ENTERED AT 16:25:35 ON 10 MAR 2009
L3            10 S L2 FULL

     FILE 'REGISTRY' ENTERED AT 16:27:34 ON 10 MAR 2009
L4             STRUCTURE UPLOADED
L5             6 S L4 FULL

     FILE 'CAPLUS' ENTERED AT 16:28:26 ON 10 MAR 2009
L6             6 S L5 FULL

     FILE 'REGISTRY' ENTERED AT 16:30:33 ON 10 MAR 2009
L7             STRUCTURE UPLOADED
L8            74 S L7 FULL

     FILE 'CAPLUS' ENTERED AT 16:31:15 ON 10 MAR 2009
L9             8 S L8 FULL

     FILE 'REGISTRY' ENTERED AT 16:34:04 ON 10 MAR 2009
L10            STRUCTURE UPLOADED
L11            6 S L10 FULL

     FILE 'CAPLUS' ENTERED AT 16:35:00 ON 10 MAR 2009
L12            2 S L11 FULL
L13           16 S L12 OR L9 OR L6 OR L3

=> log y
COST IN U.S. DOLLARS                            SINCE FILE      TOTAL
                                                   ENTRY    SESSION
FULL ESTIMATED COST                                92.74     843.66

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)      SINCE FILE      TOTAL
                                                   ENTRY    SESSION
CA SUBSCRIBER PRICE                               -13.12     -13.12

STN INTERNATIONAL LOGOFF AT 16:38:02 ON 10 MAR 2009
```